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Application Research of GMRES Algorithm in dynamic light scattering Particles Size Distribution Inversion

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Abstract

For ill-posed inversion problem of dynamic light scattering (DLS), this paper is discusses DLS inversion of GMRES algorithm. Combining Tikhonov regularization inversion strategy with GMRES algorithm, a GMRES-TIK inversion algorithm is designed in this paper. The simulation datum was respectively inversed by two methods. The inversion results demonstrate that, correct inversion results can't obtained by GMRES algorithm, however inversion results of GMRES-TIK algorithm is reasonable under a certain noise level. Therefore, we can draw conclusions that GMRES algorithm can't directly used for DLS inversion, after combining Tikhonov regularization method, it can used for DLS inversion and has strong noise immunity.

Keyword:dynamic light scattering; particle size distribution; Tikhonov regularization; GMRES; inversion.

1. Introduction

Particles measurement technique of dynamic light scattering (DLS) is an effective way to obtain the information of the sub-micron and nano-particles size [1-2]. In this technology, inversing particles size distribution (PSD) from the autocorrelation function (ACF) of scattered light intensity is an ill-posed problem, which has been a difficulty in DLS technology. According to DLS inversion principle, inversion problem of DLS are virtually a problem on optimizing parameters from measurement ACF. It need solve a large linear equations. GMRES algorithm is one of the most effective iterative methods to solve large sparse non-symmetric linear equations[3].But DLS inversion problem is an ill-posed problem.The obtained inversion results by directly solving equations by GMRES algorithm is incorrect. Tikhonov

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regularization is an popular method for solving this kind problem [4]. Therefore, this paper presents a DLS inversion algorithm which combining GMRES algorithm and Tikhonov regularization(GMRES-TIK).Numerical simulations show this algorithm has the advantages over GMRES algorithm.

2. DLS Particles Inversion Knowledge

2.1 DLS Particles Measurement Theory

For the Gaussian distribution of the light field, ACF of scattered light intensity is obtained by a Siegert relationship. For the polydisperse solutions, the normalized ACF of scattered light intensity is expressed as

$$g(\tau) = \int_0^\infty G(\Gamma)\exp(-2\Gamma\tau)d\Gamma \quad \int_0^\infty G(\Gamma)d\Gamma = 1 \qquad (1)$$

Where τ is the decay time, $\Gamma = Dq^2$ is the decay rate, $G(\Gamma)$ is normalized distribution function of the decay rate.

The decay rate is calculated by

$$\Gamma = Dq^2 \qquad (2)$$

Where D is diffusion coefficient, q is defined as

$$q = \frac{4\pi n}{\lambda}\sin(\frac{\theta}{2}) \qquad (3)$$

Where n is the refractive index of the solvent, λ is the wavelength of the incident light in vacuum, θ is scattering angle.

From the measured value of D, the radius of the particle d is calculated using the Stokes-Einstein relationship

$$D = \frac{k_B \mathrm{T}}{3\pi\eta d} \qquad (4)$$

Where k_B , T, and η are the Boltzmann constant, absolute temperature, and solvent viscosity, respectively.

According to PCS measuring principle, as long as $G(\Gamma)$ is retrieved by inversing from Eq.(1) and PSD can be know.

2.2 Inversion Theory

The discrete form of Eq. (1) can be expressed as

$$g(\tau) = \sum_{i=1}^{N} G(\Gamma_i)\exp(-2\Gamma_i\tau) \qquad (5)$$

Eq.(5) can be expressed as

$$Ax = \mathrm{b} \qquad (6)$$

where $b_j = g(\tau_j)$ $x_i = G(\Gamma_i)$, $a_{i,j} = \exp(-2\Gamma_i \tau_j)$ is an element of matrix A.

From Eq.6), PSD can be obtained by various methods of solving equations.

Considering ill condition of the equation (6), By Tikhonov Regularization method, Eq.(6) is expressed as follows

$$(A^T A + \lambda I)x = A^T b \quad (7)$$

Where λ is regularization parameter.

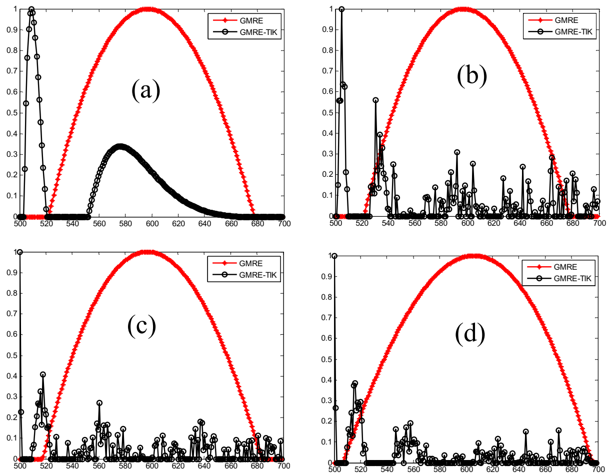

Fig.1. PSD of 600nm particles with different noise levels (a) 0, (b) 0.0001,(c) 0.001, (d)0.01

Making $(A^T A + \lambda I) = A_1$ $A^T b = b_1$, then Eq.(7) is expressed as

$$A_1 x = b_1 \quad (8)$$

Choosing regularization parameter and satisfying inequality constraints $x \geq 0$, PSD can be retrieved. In this paper, equations were solved by GMRES algorithm

3. GMRES Algorithm Theory

The GMRES method by Saad and Schultz is one of the most popular iterative solvers for large unsymmetric linear system of equations. Let x_0 be initial iterative value, $r_0 = b - Ax_0$ and $\{v_1, v_2 \cdots, v_m\}$ be an orthonormal basis of the Krylov subspace produced by Arnoldi procedure, then the key to GMRES is the implementation of the solution of the least square problem [5]

$$J(y) = \left\| \|r_0\| e_1 - \overline{H}_m y \right\|, \quad y \in R^m \quad (9)$$

where $J(y) = \overline{H}_m \in R^{(m+1)\times m}$ is an upper Hessenberg matrix. It is expressed as

$$\overline{H}_m=\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1,(m-1)} & h_{1,m} \\ h_{21} & h_{22} & \cdots & h_{2,(m-1)} & h_{2,m} \\ 0 & h_{32} & \cdots & h_{3,(m-1)} & h_{3,m} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & h_{(m-1),m} & h_{m,m} \\ 0 & 0 & \cdots & 0 & h_{(m+1),m} \end{bmatrix}$$

Letting $V_m = \{v_1, v_2 \cdots, v_m\}$, we have following formula

$$AV_m = V_{m+1}\overline{H}_m \quad (10)$$

According to formula (10) , formula (9) can be solved

4. Inversion and Analysis

In order to research application of GMRES algorithm in DLS particles size distribution inversion, simulation ACF was inversed by the GMRES and GMRES-Tikhonov algorithm. In simulation experiment, ACF is obtained according to Eq.(5). Experiment particles are respectively 600nm monodisperse particles and 20nm-60nm bi-dispersed particles (two kinds particles ratio is 1:1).Simulation experiment conditions are as follows: the wavelength is 632.8nm, the refractive index of scattering medium(water) 1.331,scattering angle 90° ,absolute temperature 25℃,Botlzman constant 1.3807×10-23 J·K-1,the viscosity coefficient of water 0.89×10-3 N·S·K-1. At the same time, in order to verify anti-noise ability of algorithm, the noises with different noise level are added to the simulated ACF. regularization parameter λ is 0.0001 in inversion. The PSD and data of two kinds of particles are shown in Fig.1, Fig.2, Table 1.

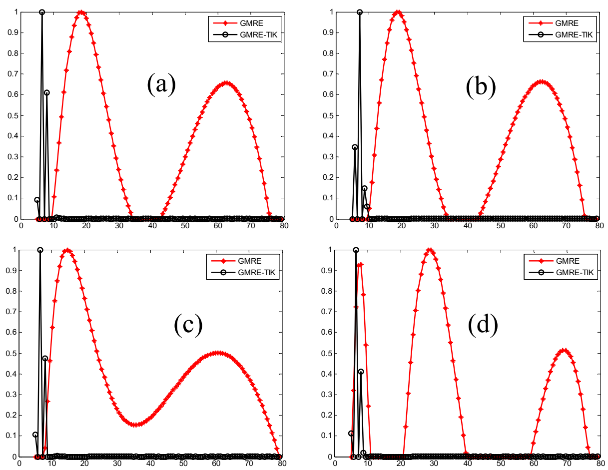

Fig.2. PSD of 20nm-60nm particles PSD with different noise levels (a) 0, (b) 0.0001,(c) 0.001, (d)0.01

Table 1 inversion size data of 600nm, 20nm-60nm particles

noise level	unimodal distribution particles	bimodal distribution particles
	peak value/nm	*peak value/nm*
0	598	18.5,60.5
0.0001	598	18.5,62.0
0.001	597	14.5, 60.5
0.01	606	—

Form Tab.1, Fig.1 and Fig.2 shows, for 600nm monodisperse particles and 20nm-60nm bi-dispersed particles, in any noise level, GMRES method can't get correct inversion result, however, when GMRES-Tikhonov algorithm was used, inversion results of 600nm monodisperse particles is reasonable at less than 0.01 noise level. that of 20nm-60nm bi-dispersed particles is reasonable at less than 0.001 noise level, Therefore, GMRES-TIK algorithm can used for DLS inversion and GMRES algorithm can not.

5. Conclusion

For ill-posed DLS inversion problem, this paper is discusses DLS inversion of GMRES algorithm. Combining Tikhonov regularization inversion strategy with GMRES algorithm, a GMRES-TIK inversion algorithm is designed in this paper. The simulation datum of 600nm, 20nm-60nm particles was respectively inversed by two algorithms. The inversion results demonstrate that, correct inversion results can't obtained by GMRES algorithm, however inversion results of GMRES-TIK algorithm is reasonable under a certain noise level. Therefore, we can draw conclusions that GMRES algorithm can't directly used for DLS inversion, after combining Tikhonov regularization method, it can used for inversion of DLS and has strong noise immunity.

References

[1] K. Takahashi, H.Kato, T.Saito. "Precise measurement of the size of nanoparticles by dynamic light scattering with Uncertainty Analysis", Part. Part. Syst. Character,Vol.25, Mar, 2008. pp. 31-38.

[2] Y.T.Cheng. .J.Shen, W.Liu. "Normalization of Autocorrelation Function for Multiple-tau photon Correlator", Chin. J. Laser, Vol.36, Feb, 2009. pp. 444-448.

[3].ZHANG Kecun，ZHAO Yingliang. "Algorithms and analysis preconditioned GMRES algorithm",SIAM J Sci Comput，

for numerical methods,1rd ed. Beijing: Science Press, 2004

[4] Liu.J.J, " Ill-posed problem of the regularization method and its application", 1rd ed. Beijing: Science Press, 2005.

[5] U H¨amarik,U Tautenhahn, "On the monotone error rule for paramter choice in iterative and continulus regularization methods",BIT, Vol.41, May, 2001. pp. 11029-1038